

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 4.47 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.63e-01

Confidence level: 7.33e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Dalapon</div> <div>Measured: 2.51</div> <div>Predicted: 2.04</div>	<div>Image not found</div> <div>Dalapon-sodium</div> <div>Measured: 1.00</div> <div>Predicted: 2.04</div>	<div>Image not found</div> <div>3-Pyridinecarbonitrile</div> <div>Measured: 36.3</div> <div>Predicted: 25.0</div>
<div>Image not found</div> <div>Epichlorohydrin</div> <div>Measured: 10.0</div> <div>Predicted: 9.87</div>	<div>Image not found</div> <div>2,2,2-Trichloroacetamide</div> <div>Measured: 9.77</div> <div>Predicted: 6.26</div>	